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DTU Energy
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The "Go Big or Go Home" Club:

Molecular Dynamics Modelling of Bulk Heterojunctions

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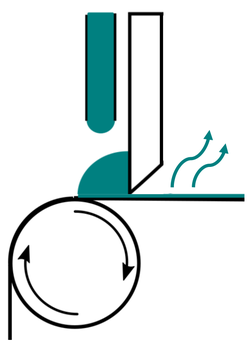
Motivation

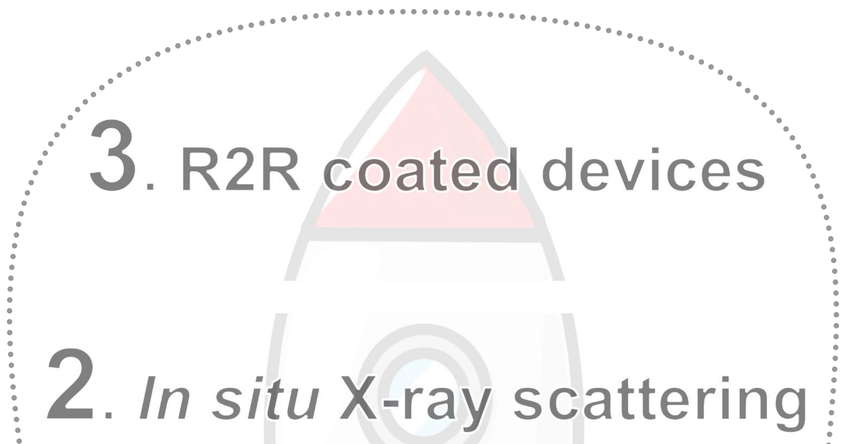
The "Go Big or Go Home" club is a collaboration within the SEEWHI H2020 project which aims upscale the manufacturing of organic photovoltaics (OPVs) without compromising the device efficiency. Usually, the efficiency is halved when moving from non-scalable spin-coating to roll-to-roll (R2R) deposition techniques, but combining the strengths of molecular dynamics (MD) modelling and *in situ* X-ray scattering enables the analysis of blend microstructure formation during post-deposition drying, in turn allowing us to identify the processing parameters that are key to overcome the scalability lag and move towards cheap, large-scale, and non-toxic solar cells with record efficiencies.

Simulating post-deposition drying

The efficiency of solution processed OPVs is crucially dependent on the 3D mesoscale thin-film morphology, which in turn is greatly influenced by solvent properties and evaporation rate.



In order to reliably simulate active layer morphologies from MD simulations, we have scripted a range of evaporation schemes incorporating e.g. potential walls mimicking substrate– and air interfaces as well as including a suspended solvent vapour above the film from which solvent molecules are continuously removed.[1]



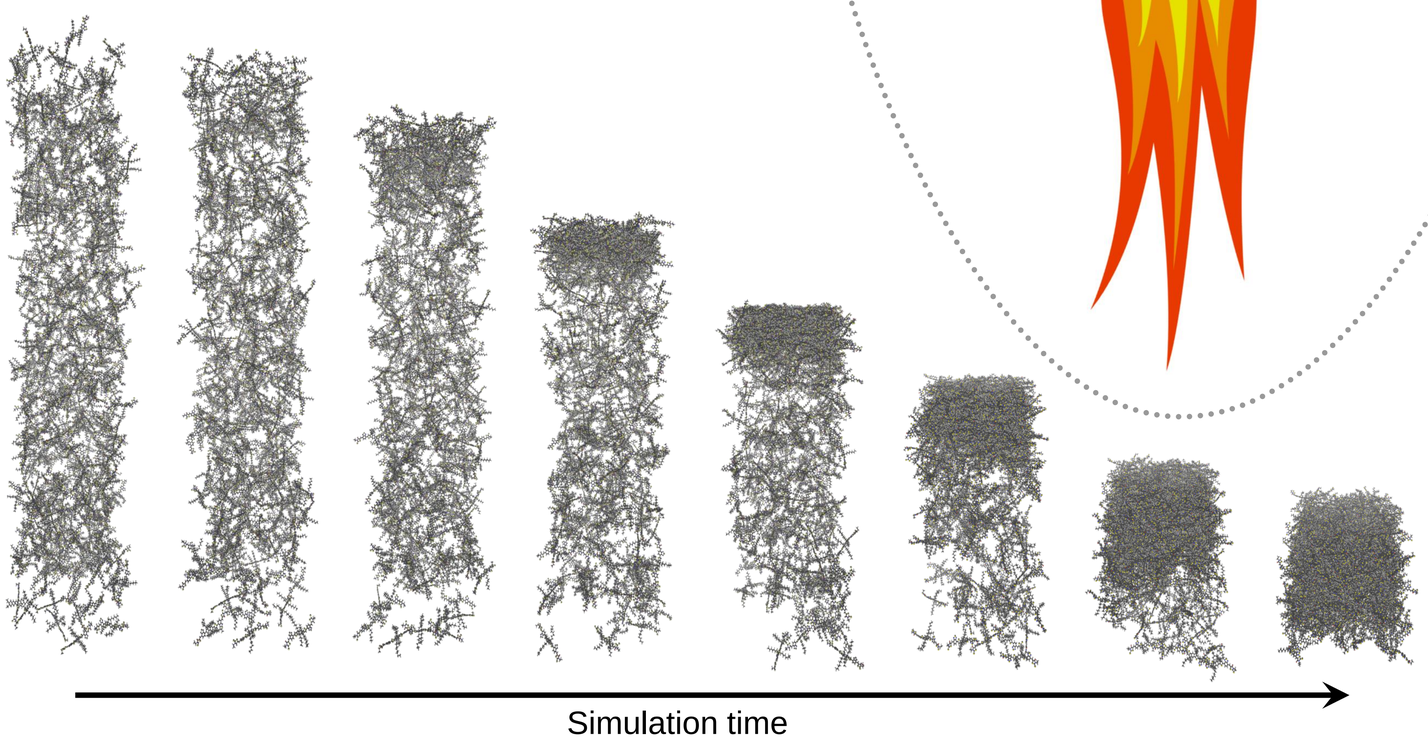


Figure 1: Solvent evaporation simulation of all-atom O-IDTBR small-molecule acceptors in coarse-grained chloroform.

Approaching experimental time-scales

Using the MARTINI force field[2] to coarse-grain our systems, the time- and length-scales relevant for morphology evolution are within reach of MD simulations:[3,4]

~1000 times speed-up

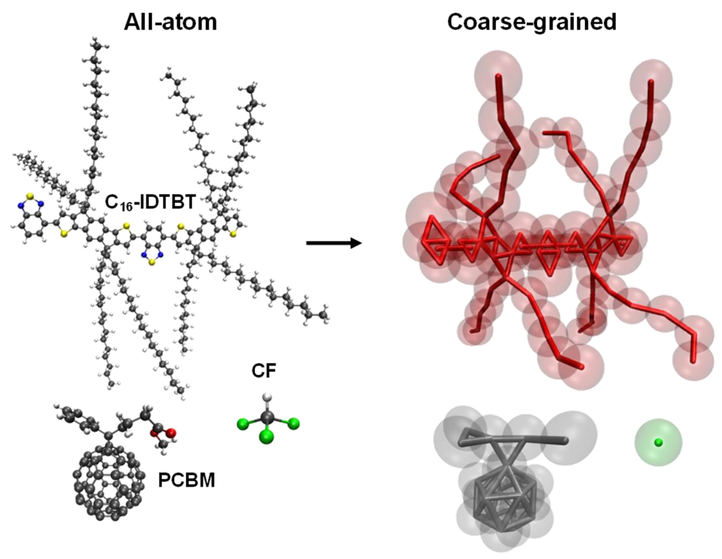


Figure 2: All-atom and MARTINI coarse-grained models for chloroform (CF), PCBM,[4] and a dimer of C_{16}-IDTBT.

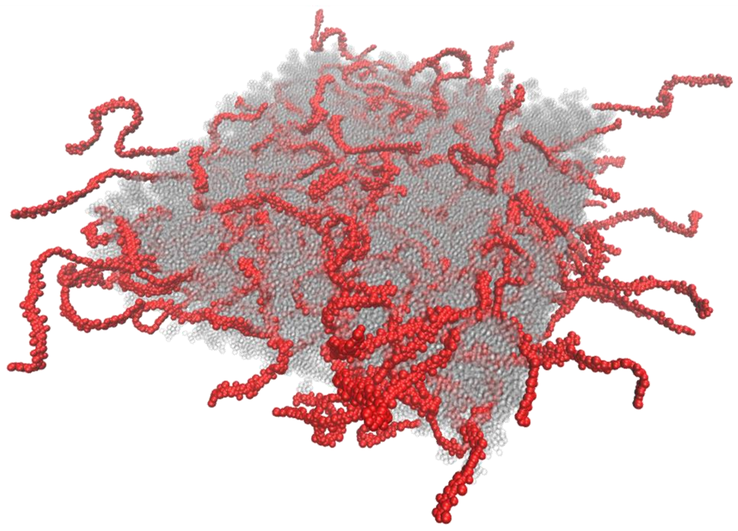


Figure 3: Thin-film of C_{16}-IDTBT 12mers (red) and PCBM (semi-transparent grey) annealed at 600 K and cooled down to 300 K. Sidechains are not shown.

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Methodology

We have used the GROMACS 2016.3 package[5] for all MD simulations. The OPLS-AA force field[6] formed the basis for the all atom simulations of IDTBT and O-IDTBR with our own parameterizations of e.g. most angles and in particular the IDT-BT torsional potential and sidechain couplings – these were based on quantum chemical DFT calculations. The coarse-grained simulations were based on the MARTINI force field[2] and in part Ref. 4.

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